



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:24 PM GMT

PDB ID : 4LJ2
Title : Crystal structure of chorismate synthase from *Acinetobacter baumannii* at 3.15Å resolution
Authors : Chaudhary, A.; Singh, N.; Kaushik, S.; Tyagi, T.K.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2013-07-04
Resolution : 3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

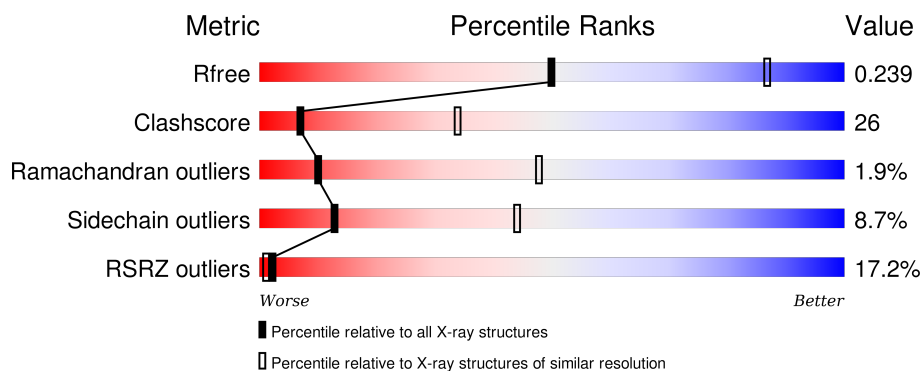
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	363	<div> <div>15%</div> <div>49%</div> <div>32%</div> <div>7%</div> <div>11%</div> </div>
1	B	363	<div> <div>16%</div> <div>50%</div> <div>35%</div> <div>•</div> <div>11%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4840 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

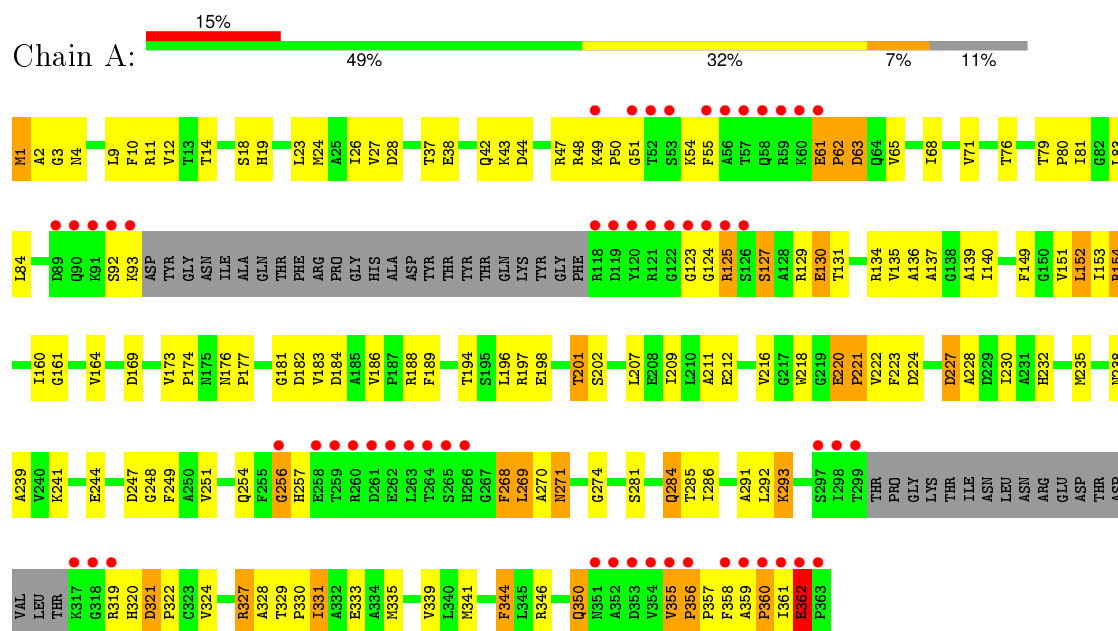
- Molecule 1 is a protein called Chorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2413	1510	437	455	11			
1	B	324	Total	C	N	O	S	0	0	0
			2427	1518	439	459	11			

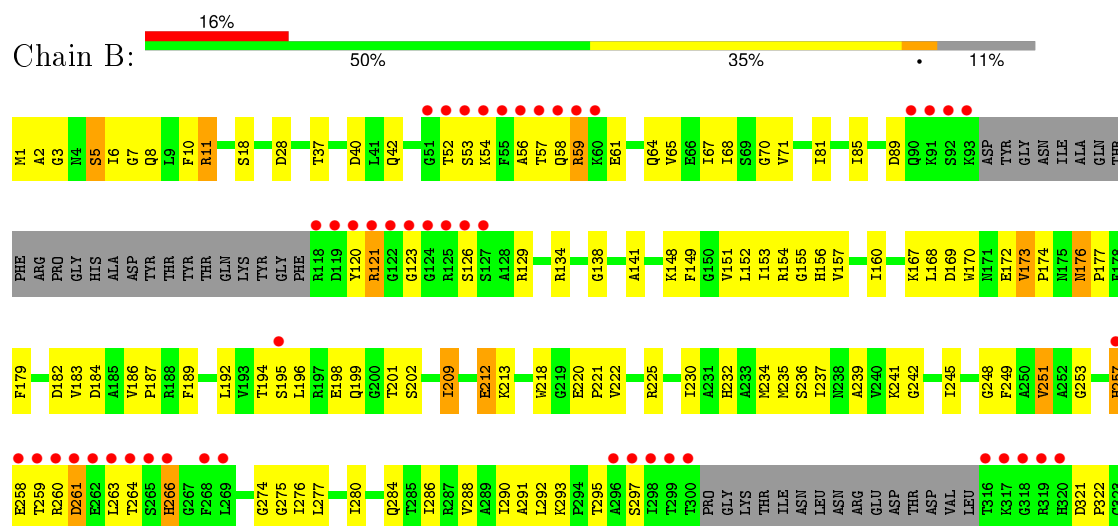
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Chorismate synthase



• Molecule 1: Chorismate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.77Å 72.61Å 89.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.54 – 3.15 46.54 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.54-3.15) 99.8 (46.54-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.252 0.223 , 0.239	Depositor DCC
R_{free} test set	654 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 12779 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4840	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.85	1/2455 (0.0%)	0.95	8/3316 (0.2%)
1	B	0.79	1/2469 (0.0%)	0.87	1/3336 (0.0%)
All	All	0.82	2/4924 (0.0%)	0.91	9/6652 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	TRP	NE1-CE2	-5.82	1.29	1.37
1	B	220	GLU	CD-OE1	-5.74	1.19	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	355	VAL	C-N-CD	-8.55	101.78	120.60
1	A	355	VAL	C-N-CD	-6.60	106.08	120.60
1	A	270	ALA	N-CA-C	-5.73	95.53	111.00
1	A	10	PHE	N-CA-C	-5.43	96.33	111.00
1	A	362	GLU	C-N-CD	-5.42	108.67	120.60
1	A	3	GLY	N-CA-C	-5.30	99.86	113.10
1	A	319	ARG	N-CA-C	-5.09	97.26	111.00
1	A	26	ILE	N-CA-C	-5.04	97.39	111.00
1	A	61	GLU	C-N-CD	-5.01	109.58	120.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	GLY	Peptide
1	A	269	LEU	Peptide
1	A	321	ASP	Peptide
1	B	59	ARG	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2413	0	2422	145	0
1	B	2427	0	2436	135	0
All	All	4840	0	4858	257	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (257) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:VAL:HB	1:A:356:PRO:HD2	1.25	1.13
1:B:173:VAL:HG22	1:B:174:PRO:HD3	1.37	1.04
1:A:358:PHE:CE2	1:A:361:ILE:HD11	1.94	1.02
1:A:331:ILE:O	1:A:331:ILE:HG13	1.60	1.01
1:A:251:VAL:HG11	1:B:293:LYS:HB3	1.44	0.99
1:A:359:ALA:HB1	1:A:360:PRO:HD2	1.41	0.99
1:A:355:VAL:HB	1:A:356:PRO:CD	1.95	0.96
1:A:18:SER:HB2	1:A:125:ARG:HB3	1.51	0.92
1:A:355:VAL:CB	1:A:356:PRO:HD2	1.99	0.91
1:A:18:SER:HB2	1:A:125:ARG:CB	2.03	0.88
1:B:195:SER:O	1:B:198:GLU:HB2	1.74	0.88
1:B:321:ASP:HB3	1:B:324:VAL:HG13	1.55	0.86
1:B:68:ILE:HG22	1:B:68:ILE:O	1.77	0.84
1:A:251:VAL:CG1	1:B:293:LYS:HB3	2.09	0.83
1:A:327:ARG:O	1:A:330:PRO:HD2	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:ALA:N	1:B:360:PRO:CD	2.43	0.81
1:B:248:GLY:O	1:B:251:VAL:HB	1.82	0.80
1:A:54:LYS:HE3	1:A:177:PRO:HB3	1.63	0.80
1:A:358:PHE:CE2	1:A:361:ILE:CD1	2.65	0.79
1:B:359:ALA:N	1:B:360:PRO:HD3	1.97	0.79
1:A:331:ILE:O	1:A:331:ILE:CG1	2.29	0.79
1:B:57:THR:CG2	1:B:57:THR:O	2.30	0.79
1:A:293:LYS:HA	1:B:251:VAL:HG13	1.65	0.79
1:A:232:HIS:HB2	1:B:232:HIS:HB2	1.65	0.78
1:B:58:GLN:HG3	1:B:59:ARG:N	1.99	0.78
1:A:221:PRO:O	1:B:2:ALA:HA	1.84	0.78
1:B:173:VAL:HG22	1:B:174:PRO:CD	2.14	0.77
1:B:334:ALA:O	1:B:338:ILE:HG12	1.84	0.77
1:A:269:LEU:HD13	1:A:284:GLN:NE2	2.01	0.75
1:A:251:VAL:CG1	1:B:293:LYS:CB	2.64	0.75
1:A:271:ASN:HD21	1:A:284:GLN:CD	1.91	0.75
1:B:89:ASP:OD1	1:B:129:ARG:NH2	2.20	0.74
1:A:201:THR:HG22	1:A:202:SER:H	1.51	0.74
1:B:70:GLY:HA3	1:B:81:ILE:HD13	1.70	0.74
1:A:127:SER:HB2	1:A:130:GLU:HG2	1.71	0.73
1:A:92:SER:O	1:A:93:LYS:HB2	1.88	0.73
1:A:1:MET:O	1:A:2:ALA:HB2	1.89	0.73
1:A:268:PHE:CD1	1:A:268:PHE:N	2.54	0.72
1:A:324:VAL:HG13	1:A:324:VAL:O	1.90	0.72
1:B:57:THR:O	1:B:57:THR:HG22	1.89	0.71
1:A:127:SER:HA	1:A:129:ARG:HG3	1.74	0.70
1:A:362:GLU:HG2	1:A:362:GLU:O	1.92	0.70
1:B:230:ILE:HD12	1:B:336:LEU:HD12	1.72	0.70
1:B:126:SER:OG	1:B:129:ARG:HG3	1.92	0.70
1:A:131:THR:HG22	1:A:131:THR:O	1.92	0.70
1:A:196:LEU:HD22	1:A:201:THR:HB	1.74	0.70
1:A:251:VAL:CG1	1:B:293:LYS:HA	2.23	0.69
1:B:359:ALA:H	1:B:360:PRO:HD3	1.56	0.69
1:A:251:VAL:HG11	1:B:293:LYS:CB	2.21	0.68
1:A:92:SER:O	1:A:93:LYS:CB	2.43	0.67
1:A:251:VAL:CG1	1:B:293:LYS:CA	2.73	0.66
1:B:68:ILE:CG2	1:B:68:ILE:O	2.43	0.66
1:B:53:SER:O	1:B:54:LYS:HB2	1.93	0.66
1:A:359:ALA:HB1	1:A:360:PRO:CD	2.24	0.66
1:B:170:TRP:O	1:B:173:VAL:HG13	1.96	0.66
1:B:183:VAL:HG13	1:B:184:ASP:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:CD1	1:A:284:GLN:NE2	2.61	0.64
1:A:355:VAL:CB	1:A:356:PRO:CD	2.66	0.64
1:A:182:ASP:C	1:A:182:ASP:OD1	2.30	0.64
1:A:328:ALA:O	1:A:331:ILE:HG23	1.97	0.64
1:B:173:VAL:CG2	1:B:174:PRO:HD3	2.23	0.64
1:A:227:ASP:N	1:A:227:ASP:OD1	2.29	0.64
1:A:268:PHE:N	1:A:268:PHE:HD1	1.95	0.64
1:A:131:THR:HG23	1:A:331:ILE:CD1	2.28	0.63
1:A:251:VAL:HG12	1:B:293:LYS:HA	1.81	0.63
1:A:152:LEU:O	1:A:153:ILE:HD13	1.98	0.63
1:A:269:LEU:HG	1:A:269:LEU:O	1.99	0.63
1:B:152:LEU:HD13	1:B:154:ARG:HD2	1.82	0.61
1:A:131:THR:HG23	1:A:331:ILE:HD12	1.81	0.61
1:B:67:ILE:HG21	1:B:71:VAL:HG22	1.83	0.61
1:A:329:THR:O	1:A:333:GLU:HG3	1.99	0.60
1:B:324:VAL:HG12	1:B:327:ARG:HH12	1.67	0.60
1:B:7:GLY:O	1:B:11:ARG:HG3	2.01	0.60
1:A:42:GLN:OE1	1:A:65:VAL:HG12	2.02	0.59
1:A:19:HIS:HB3	1:A:124:GLY:HA2	1.83	0.59
1:A:212:GLU:HA	1:A:285:THR:HG22	1.84	0.59
1:A:131:THR:HG22	1:A:135:VAL:HG23	1.84	0.58
1:A:274:GLY:O	1:A:286:ILE:HA	2.04	0.58
1:B:350:GLN:C	1:B:351:ASN:HD22	2.06	0.58
1:B:274:GLY:O	1:B:286:ILE:HA	2.04	0.58
1:B:61:GLU:CD	1:B:61:GLU:H	2.04	0.58
1:A:207:LEU:HD13	1:A:292:LEU:CD1	2.34	0.58
1:A:211:ALA:HB3	1:A:286:ILE:HB	1.85	0.57
1:B:239:ALA:O	1:B:292:LEU:HA	2.03	0.57
1:B:192:LEU:O	1:B:196:LEU:HG	2.04	0.57
1:B:138:GLY:HA2	1:B:338:ILE:HD13	1.88	0.56
1:A:152:LEU:HD13	1:A:154:ARG:CZ	2.36	0.56
1:B:361:ILE:O	1:B:361:ILE:HD12	2.06	0.56
1:A:220:GLU:O	1:A:224:ASP:C	2.45	0.55
1:A:359:ALA:CB	1:A:360:PRO:HD2	2.26	0.55
1:A:51:GLY:HA3	1:A:54:LYS:HB2	1.89	0.55
1:A:269:LEU:HD13	1:A:284:GLN:HE21	1.72	0.55
1:B:153:ILE:N	1:B:153:ILE:HD12	2.22	0.55
1:B:141:ALA:HB1	1:B:341:MET:HB2	1.87	0.55
1:B:18:SER:HA	1:B:129:ARG:HD2	1.90	0.54
1:A:251:VAL:HG13	1:B:293:LYS:CB	2.37	0.54
1:A:54:LYS:CE	1:A:177:PRO:HB3	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HD13	1:A:84:LEU:HB3	1.89	0.54
1:A:136:ALA:O	1:A:140:ILE:HD12	2.07	0.54
1:A:320:HIS:O	1:A:322:PRO:HD3	2.07	0.54
1:A:350:GLN:HG2	1:B:1:MET:SD	2.48	0.54
1:B:230:ILE:HD12	1:B:336:LEU:CD1	2.38	0.54
1:A:127:SER:C	1:A:129:ARG:H	2.07	0.53
1:B:230:ILE:CD1	1:B:336:LEU:HD12	2.37	0.53
1:A:182:ASP:OD1	1:A:184:ASP:N	2.41	0.53
1:A:12:VAL:HG22	1:A:27:VAL:HG13	1.89	0.53
1:B:70:GLY:CA	1:B:81:ILE:HD13	2.39	0.53
1:B:261:ASP:HB3	1:B:263:LEU:HG	1.91	0.53
1:B:276:ILE:HD12	1:B:276:ILE:N	2.24	0.53
1:A:18:SER:HB2	1:A:125:ARG:HB2	1.85	0.52
1:B:295:THR:HG21	1:B:324:VAL:HG21	1.90	0.52
1:B:321:ASP:HB2	1:B:322:PRO:CA	2.39	0.52
1:B:61:GLU:O	1:B:61:GLU:HG2	2.09	0.52
1:A:207:LEU:HD13	1:A:292:LEU:HD13	1.91	0.52
1:A:81:ILE:N	1:A:81:ILE:HD12	2.24	0.52
1:A:43:LYS:O	1:A:47:ARG:HG3	2.09	0.52
1:B:245:ILE:CD1	1:B:288:VAL:HB	2.40	0.52
1:B:186:VAL:HB	1:B:187:PRO:CD	2.39	0.52
1:B:170:TRP:HA	1:B:173:VAL:CG1	2.38	0.52
1:A:209:ILE:HD12	1:A:209:ILE:N	2.24	0.52
1:A:160:ILE:HD11	1:A:189:PHE:CD2	2.44	0.52
1:B:56:ALA:O	1:B:57:THR:HB	2.09	0.52
1:A:19:HIS:CD2	1:A:19:HIS:H	2.27	0.52
1:A:18:SER:CB	1:A:125:ARG:HB2	2.40	0.51
1:B:183:VAL:CG1	1:B:184:ASP:N	2.73	0.51
1:A:127:SER:C	1:A:129:ARG:N	2.57	0.51
1:B:67:ILE:HG21	1:B:71:VAL:CG2	2.41	0.51
1:A:238:ASN:HA	1:B:225:ARG:HH12	1.76	0.51
1:A:293:LYS:HA	1:B:251:VAL:CG1	2.39	0.51
1:A:291:ALA:HB2	1:B:249:PHE:CD1	2.46	0.51
1:B:324:VAL:HG12	1:B:327:ARG:NH1	2.25	0.50
1:A:216:VAL:HG23	1:A:281:SER:O	2.11	0.50
1:A:131:THR:CG2	1:A:131:THR:O	2.58	0.50
1:A:241:LYS:HE3	1:B:245:ILE:O	2.11	0.50
1:B:218:TRP:CH2	1:B:344:PHE:HB2	2.46	0.50
1:A:61:GLU:HB2	1:A:62:PRO:O	2.11	0.50
1:B:259:THR:HG21	1:B:263:LEU:HB2	1.94	0.50
1:B:351:ASN:HD22	1:B:351:ASN:N	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ASP:HB3	1:A:324:VAL:HB	1.93	0.50
1:A:183:VAL:HG13	1:A:184:ASP:N	2.25	0.50
1:A:11:ARG:HG2	1:A:28:ASP:HB2	1.93	0.50
1:B:354:VAL:HG12	1:B:355:VAL:O	2.12	0.50
1:B:10:PHE:HA	1:B:28:ASP:O	2.12	0.50
1:B:154:ARG:NH1	1:B:212:GLU:OE2	2.45	0.49
1:A:238:ASN:O	1:A:239:ALA:HB3	2.12	0.49
1:B:295:THR:HG21	1:B:324:VAL:CG2	2.41	0.49
1:B:148:LYS:HG2	1:B:149:PHE:CE2	2.47	0.49
1:B:59:ARG:O	1:B:59:ARG:HG3	2.11	0.49
1:B:120:TYR:HD1	1:B:121:ARG:HG3	1.77	0.49
1:A:1:MET:O	1:A:2:ALA:CB	2.54	0.49
1:B:353:ASP:N	1:B:353:ASP:OD2	2.44	0.49
1:A:153:ILE:HD13	1:A:211:ALA:HA	1.92	0.49
1:B:173:VAL:CG2	1:B:174:PRO:CD	2.86	0.49
1:B:276:ILE:HD11	1:B:286:ILE:HG23	1.94	0.49
1:B:234:MET:O	1:B:237:ILE:HD12	2.13	0.49
1:B:160:ILE:HD12	1:B:189:PHE:CD2	2.48	0.49
1:A:328:ALA:O	1:A:331:ILE:CG2	2.61	0.48
1:A:222:VAL:HG11	1:B:134:ARG:CZ	2.43	0.48
1:A:71:VAL:HG12	1:A:76:THR:HA	1.95	0.48
1:A:4:ASN:HB2	1:A:14:THR:O	2.12	0.48
1:A:248:GLY:O	1:A:251:VAL:HG23	2.12	0.48
1:B:153:ILE:HG23	1:B:336:LEU:HD23	1.95	0.48
1:B:277:LEU:O	1:B:280:ILE:HG13	2.14	0.48
1:A:173:VAL:HG22	1:A:174:PRO:HD3	1.95	0.48
1:A:221:PRO:HA	1:A:222:VAL:C	2.34	0.48
1:A:49:LYS:HD3	1:A:55:PHE:HZ	1.79	0.47
1:B:57:THR:O	1:B:57:THR:HG23	2.12	0.47
1:B:54:LYS:HD3	1:B:54:LYS:HA	1.65	0.47
1:B:155:GLY:HA2	1:B:209:ILE:HA	1.96	0.47
1:A:62:PRO:HB2	1:A:63:ASP:H	1.39	0.47
1:A:131:THR:HG22	1:A:135:VAL:CG2	2.45	0.47
1:A:152:LEU:HD22	1:A:154:ARG:CD	2.45	0.47
1:B:149:PHE:HB2	1:B:151:VAL:HG23	1.97	0.47
1:A:161:GLY:O	1:B:253:GLY:HA2	2.14	0.47
1:A:223:PHE:HB2	1:B:3:GLY:O	2.15	0.47
1:A:23:LEU:HD11	1:A:129:ARG:HB3	1.97	0.47
1:B:169:ASP:O	1:B:172:GLU:HB3	2.15	0.47
1:B:167:LYS:HE2	1:B:182:ASP:OD1	2.15	0.47
1:A:176:ASN:HB2	1:A:177:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:OE1	1:A:38:GLU:N	2.48	0.46
1:A:9:LEU:HD12	1:A:346:ARG:HA	1.98	0.46
1:A:152:LEU:HD22	1:A:154:ARG:HD2	1.97	0.46
1:B:170:TRP:HA	1:B:173:VAL:HG13	1.96	0.46
1:A:173:VAL:HG12	1:A:181:GLY:HA2	1.98	0.46
1:B:172:GLU:O	1:B:176:ASN:ND2	2.48	0.46
1:A:256:GLY:O	1:A:257:HIS:CG	2.68	0.46
1:B:292:LEU:HD22	1:B:325:GLY:HA2	1.98	0.46
1:A:230:ILE:HA	1:A:339:VAL:HG21	1.99	0.45
1:B:37:THR:O	1:B:40:ASP:HB2	2.17	0.45
1:A:131:THR:HG23	1:A:331:ILE:HD13	1.98	0.45
1:B:257:HIS:O	1:B:257:HIS:ND1	2.40	0.45
1:B:5:SER:OG	1:B:6:ILE:N	2.48	0.45
1:A:153:ILE:CD1	1:A:211:ALA:HA	2.46	0.45
1:B:138:GLY:HA2	1:B:338:ILE:CD1	2.46	0.45
1:A:355:VAL:O	1:A:356:PRO:O	2.35	0.44
1:B:321:ASP:CB	1:B:324:VAL:HG13	2.38	0.44
1:B:156:HIS:CE1	1:B:168:LEU:HD13	2.52	0.44
1:A:355:VAL:O	1:A:356:PRO:C	2.55	0.44
1:B:170:TRP:C	1:B:173:VAL:HG13	2.37	0.44
1:B:222:VAL:HG23	1:B:222:VAL:H	1.36	0.44
1:A:244:GLU:HA	1:B:242:GLY:HA2	2.00	0.44
1:A:50:PRO:O	1:A:54:LYS:HE2	2.18	0.44
1:A:271:ASN:ND2	1:A:284:GLN:CD	2.67	0.44
1:A:61:GLU:N	1:A:62:PRO:HA	2.32	0.44
1:B:258:GLU:OE1	1:B:260:ARG:CZ	2.65	0.44
1:B:212:GLU:O	1:B:213:LYS:HB2	2.17	0.44
1:A:320:HIS:O	1:A:322:PRO:CD	2.66	0.44
1:B:354:VAL:O	1:B:356:PRO:HD3	2.17	0.44
1:A:173:VAL:HG12	1:A:181:GLY:CA	2.48	0.44
1:A:134:ARG:HD2	1:A:335:MET:CE	2.48	0.44
1:A:24:MET:HA	1:A:83:LEU:O	2.18	0.44
1:B:321:ASP:HB2	1:B:322:PRO:HA	1.99	0.43
1:B:157:VAL:HG21	1:B:326:VAL:HG12	2.00	0.43
1:A:358:PHE:CZ	1:A:361:ILE:HD12	2.53	0.43
1:B:329:THR:HB	1:B:330:PRO:HD3	2.00	0.43
1:A:48:ARG:O	1:A:50:PRO:HD3	2.18	0.43
1:B:65:VAL:HA	1:B:85:ILE:HG13	2.01	0.43
1:A:362:GLU:O	1:A:362:GLU:CG	2.63	0.43
1:A:341:MET:O	1:A:344:PHE:HB3	2.18	0.43
1:A:68:ILE:CD1	1:A:84:LEU:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ASN:C	1:B:177:PRO:O	2.57	0.43
1:A:149:PHE:HB2	1:A:151:VAL:HG23	2.01	0.43
1:B:42:GLN:OE1	1:B:64:GLN:HA	2.19	0.43
1:B:173:VAL:CG2	1:B:174:PRO:N	2.81	0.42
1:B:292:LEU:CD2	1:B:325:GLY:HA2	2.50	0.42
1:B:275:GLY:C	1:B:276:ILE:HD12	2.40	0.42
1:B:266:HIS:HD2	1:B:266:HIS:O	2.02	0.42
1:B:202:SER:HA	1:B:322:PRO:O	2.20	0.42
1:A:137:ALA:HA	1:A:140:ILE:CD1	2.49	0.42
1:A:194:THR:O	1:A:198:GLU:HG2	2.19	0.42
1:A:18:SER:CB	1:A:125:ARG:CB	2.86	0.42
1:A:136:ALA:O	1:A:139:ALA:HB3	2.20	0.42
1:B:331:ILE:HD12	1:B:331:ILE:N	2.34	0.42
1:B:290:ILE:HD12	1:B:292:LEU:HD11	2.01	0.42
1:B:120:TYR:HA	1:B:121:ARG:HA	1.73	0.42
1:B:258:GLU:HB2	1:B:260:ARG:HG3	2.02	0.42
1:B:173:VAL:N	1:B:174:PRO:CD	2.83	0.41
1:B:53:SER:HB3	1:B:54:LYS:H	1.68	0.41
1:B:70:GLY:C	1:B:81:ILE:HD13	2.40	0.41
1:B:52:THR:O	1:B:53:SER:HB2	2.20	0.41
1:A:79:THR:HB	1:A:80:PRO:HD2	2.02	0.41
1:A:182:ASP:O	1:A:186:VAL:HG23	2.21	0.41
1:A:228:ALA:HA	1:B:235:MET:HB3	2.01	0.41
1:B:280:ILE:C	1:B:280:ILE:HD12	2.40	0.41
1:A:238:ASN:HA	1:B:225:ARG:NH1	2.34	0.41
1:A:256:GLY:O	1:A:257:HIS:ND1	2.53	0.41
1:A:247:ASP:OD1	1:A:254:GLN:NE2	2.49	0.41
1:A:249:PHE:CD1	1:B:291:ALA:HB2	2.55	0.41
1:A:137:ALA:HA	1:A:140:ILE:HD13	2.01	0.41
1:B:241:LYS:HA	1:B:241:LYS:HD2	1.77	0.41
1:A:284:GLN:H	1:A:284:GLN:HG2	1.56	0.41
1:B:230:ILE:CD1	1:B:339:VAL:HB	2.51	0.41
1:B:286:ILE:HD12	1:B:286:ILE:N	2.36	0.40
1:A:164:VAL:O	1:A:188:ARG:NH2	2.54	0.40
1:A:358:PHE:CZ	1:A:361:ILE:CD1	3.03	0.40
1:B:324:VAL:O	1:B:325:GLY:C	2.58	0.40
1:A:134:ARG:HD2	1:A:335:MET:HE3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	316/363 (87%)	288 (91%)	22 (7%)	6 (2%)	10	48
1	B	318/363 (88%)	283 (89%)	29 (9%)	6 (2%)	10	48
All	All	634/726 (87%)	571 (90%)	51 (8%)	12 (2%)	10	48

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	PRO
1	A	221	PRO
1	B	357	PRO
1	B	360	PRO
1	A	123	GLY
1	A	356	PRO
1	B	123	GLY
1	B	179	PHE
1	A	357	PRO
1	B	356	PRO
1	A	360	PRO
1	B	359	ALA

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	251/286 (88%)	227 (90%)	24 (10%)	10	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	253/286 (88%)	233 (92%)	20 (8%)	15	51
All	All	504/572 (88%)	460 (91%)	44 (9%)	13	44

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	37	THR
1	A	44	ASP
1	A	63	ASP
1	A	125	ARG
1	A	127	SER
1	A	130	GLU
1	A	152	LEU
1	A	154	ARG
1	A	169	ASP
1	A	197	ARG
1	A	201	THR
1	A	220	GLU
1	A	227	ASP
1	A	235	MET
1	A	268	PHE
1	A	271	ASN
1	A	284	GLN
1	A	293	LYS
1	A	327	ARG
1	A	331	ILE
1	A	344	PHE
1	A	350	GLN
1	A	362	GLU
1	B	5	SER
1	B	8	GLN
1	B	11	ARG
1	B	121	ARG
1	B	173	VAL
1	B	176	ASN
1	B	194	THR
1	B	199	GLN
1	B	201	THR
1	B	209	ILE
1	B	212	GLU
1	B	221	PRO

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Mol	Chain	Res	Type
1	B	236	SER
1	B	251	VAL
1	B	257	HIS
1	B	261	ASP
1	B	264	THR
1	B	266	HIS
1	B	284	GLN
1	B	297	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	175	ASN
1	A	271	ASN
1	A	284	GLN
1	B	175	ASN
1	B	176	ASN
1	B	266	HIS
1	B	351	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	322/363 (88%)	0.49	53 (16%) 2 1	3, 15, 100, 100	0
1	B	324/363 (89%)	0.60	58 (17%) 2 1	3, 21, 100, 100	0
All	All	646/726 (88%)	0.54	111 (17%) 2 1	3, 17, 100, 100	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	361	ILE	11.9
1	B	92	SER	11.3
1	B	93	LYS	10.2
1	B	261	ASP	9.6
1	A	92	SER	9.0
1	B	52	THR	8.4
1	B	264	THR	7.8
1	A	262	GLU	7.6
1	A	60	LYS	7.5
1	B	262	GLU	7.3
1	A	58	GLN	7.0
1	A	261	ASP	6.9
1	A	354	VAL	6.8
1	A	55	PHE	6.8
1	A	57	THR	6.7
1	B	58	GLN	6.6
1	B	90	GLN	6.5
1	A	126	SER	6.5
1	B	57	THR	6.5
1	A	260	ARG	6.2
1	B	53	SER	6.1
1	A	259	THR	5.9
1	B	122	GLY	5.9
1	A	59	ARG	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	363	PRO	5.7
1	A	359	ALA	5.6
1	A	56	ALA	5.3
1	B	300	THR	5.3
1	B	299	THR	5.3
1	A	362	GLU	5.3
1	B	56	ALA	5.3
1	A	360	PRO	5.2
1	B	91	LYS	5.2
1	B	360	PRO	5.2
1	B	123	GLY	5.1
1	B	357	PRO	5.0
1	B	265	SER	5.0
1	B	356	PRO	5.0
1	A	265	SER	5.0
1	B	353	ASP	4.9
1	B	297	SER	4.9
1	B	260	ARG	4.7
1	A	355	VAL	4.7
1	B	266	HIS	4.7
1	B	355	VAL	4.7
1	B	118	ARG	4.6
1	A	122	GLY	4.6
1	A	125	ARG	4.6
1	A	263	LEU	4.6
1	B	121	ARG	4.6
1	A	119	ASP	4.5
1	A	264	THR	4.5
1	A	297	SER	4.5
1	A	123	GLY	4.4
1	B	361	ILE	4.4
1	B	263	LEU	4.4
1	A	317	LYS	4.2
1	B	316	THR	4.1
1	B	126	SER	4.1
1	A	91	LYS	4.0
1	B	51	GLY	4.0
1	A	318	GLY	3.9
1	B	55	PHE	3.9
1	B	363	PRO	3.9
1	A	266	HIS	3.9
1	B	120	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	298	ILE	3.9
1	A	90	GLN	3.8
1	B	60	LYS	3.8
1	A	353	ASP	3.8
1	A	319	ARG	3.7
1	B	296	ALA	3.6
1	B	119	ASP	3.6
1	A	118	ARG	3.5
1	B	59	ARG	3.5
1	A	120	TYR	3.5
1	B	359	ALA	3.4
1	B	127	SER	3.4
1	A	93	LYS	3.4
1	A	356	PRO	3.3
1	B	354	VAL	3.3
1	B	318	GLY	3.3
1	B	319	ARG	3.2
1	B	258	GLU	3.2
1	B	269	LEU	3.2
1	B	320	HIS	3.2
1	A	49	LYS	3.2
1	B	259	THR	3.1
1	B	124	GLY	3.1
1	A	51	GLY	3.1
1	B	257	HIS	3.1
1	A	258	GLU	3.0
1	A	124	GLY	2.9
1	B	268	PHE	2.9
1	A	53	SER	2.9
1	B	54	LYS	2.7
1	A	89	ASP	2.6
1	B	358	PHE	2.6
1	B	298	ILE	2.6
1	B	317	LYS	2.5
1	A	352	ALA	2.4
1	A	299	THR	2.4
1	B	362	GLU	2.3
1	A	121	ARG	2.2
1	A	358	PHE	2.2
1	A	61	GLU	2.2
1	A	256	GLY	2.2
1	A	52	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	195	SER	2.1
1	B	125	ARG	2.1
1	A	351	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.